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Article

Physics-Informed Graph Transformer for Simulating Land-Atmosphere Coupling Processes and Extreme Precipitation Prediction

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ABSTRACT

Land-atmosphere coupling processes, involving the exchange of energy, water, and momentum between the land surface and the atmosphere, are critical for regulating regional weather systems and extreme precipitation events. Traditional land-atmosphere coupling models rely on parameterization schemes that simplify complex nonlinear processes (e.g., soil moisture-evaporation feedback, vegetation-atmosphere interaction), leading to significant uncertainties in simulating key variables such as latent heat flux, boundary layer stability, and thus extreme precipitation prediction. This study proposes a Physics-Informed Graph Transformer (PI-GT) framework for land-atmosphere coupling simulation and extreme precipitation prediction. The framework constructs a dynamic spatial-temporal graph based on the physical connections between land surface and atmospheric grid cells, and integrates physical constraints (e.g., water balance, energy conservation) into the transformer architecture to ensure physical rationality. Multi-source observation data, including satellite-derived soil moisture, vegetation index, in-situ flux tower data, and reanalysis data, are assimilated to optimize the model's representation of key coupling processes. Validation results based on 25 years of observation data from 120 flux tower sites and extreme precipitation events in major river basins of China and the United States show that the PI-GT framework improves the average simulation accuracy of key land-atmosphere coupling variables by 27% compared to the traditional Community Land Model (CLM) 5.0. For extreme precipitation prediction (24-hour lead time), the framework reduces the root mean square error (RMSE) by 29% and increases the critical success index (CSI) by 32% compared to the Weather Research and Forecasting (WRF) model's land-atmosphere coupling module. Simulation under CMIP6 SSP3-7.0 and SSP5-8.5 scenarios indicates that the PI-GT framework reduces the uncertainty of extreme precipitation frequency projection by 21-25% by the end of the 21st century. Specifically, in the Yangtze River Basin and the Mississippi River Basin, the framework accurately captures the positive feedback effect of soil moisture anomalies on extreme precipitation and the regulating effect of vegetation cover on land-atmosphere water exchange. This study provides a new approach for improving the simulation accuracy of land-atmosphere coupling processes in Earth system models and enhances the reliability of extreme precipitation prediction, offering important scientific support for formulating flood disaster prevention and mitigation strategies.

Keywords: Computational Earth System Dynamics; Physics-Informed Graph Transformer; Land-Atmosphere Coupling; Extreme Precipitation; Data Assimilation; Climate Scenario Simulation

1. Introduction

1.1 Research Background

The land surface and atmosphere form a closely coupled system through the exchange of water vapor, energy, and momentum, which is a core component of the Earth system (Li et al., 2024). Land-atmosphere coupling processes, such as soil moisture evaporation, vegetation transpiration, and boundary layer energy exchange, directly affect the formation and development of regional precipitation systems, especially extreme precipitation events (Zhang et al., 2024). Extreme precipitation, as a typical meteorological disaster, often leads to floods, landslides, and other secondary disasters, causing severe losses to human life and property (Davis et al., 2024). With the intensification of global warming, changes in land-atmosphere coupling processes (e.g., increased soil moisture variability, altered vegetation cover) have further increased the frequency and intensity of extreme precipitation events in many regions, posing greater challenges to disaster prevention and mitigation (Wilson et al., 2024).

Computational Earth system dynamics provides an effective tool for studying land-atmosphere coupling processes and their impact on extreme precipitation, relying on numerical simulation models to quantify the interaction mechanisms between the land surface and the atmosphere (Gao et al., 2024). Traditional land-atmosphere coupling models, such as the Community Land Model (CLM) and the Noah-MP model, adopt parameterization schemes to describe complex coupling processes (Oleson et al., 2023). However, these schemes have inherent limitations due to the complexity of land-atmosphere interactions and the uncertainty of physical mechanism understanding. For example, the CLM model uses a linear parameterization to describe the relationship between soil moisture and evaporation, which cannot accurately capture the nonlinear feedback effect of soil moisture on atmospheric humidity and precipitation (Chen et al., 2023). Additionally, traditional models often treat the land surface as a uniform medium, ignoring the spatial heterogeneity of vegetation cover, soil texture, and topography, leading to inaccurate simulation of local-scale land-atmosphere coupling processes and further affecting the accuracy of extreme precipitation prediction (Wang et al., 2023).

In recent years, deep learning models have been widely applied in the field of land-atmosphere simulation and precipitation prediction, providing new solutions to overcome the limitations of traditional parameterization schemes (Reichstein et al., 2024). Convolutional Neural Networks (CNNs) and Long Short-Term Memory (LSTM) networks have been used to simulate soil moisture dynamics and precipitation prediction, respectively, by capturing spatial and temporal features (Kang et al., 2023). However, these models have obvious shortcomings in capturing the non-local and dynamic spatial connections in land-atmosphere coupling processes. For example, CNNs are limited to local grid convolution and cannot effectively model the remote impact of soil moisture anomalies on precipitation systems, while LSTMs struggle to integrate the spatial dependencies between land surface variables and atmospheric variables (Guo et al., 2024). Transformer models, with their self-attention mechanism, have shown strong capabilities in capturing long-range spatial and temporal dependencies, but pure data-driven transformer models often produce unphysical results due to the lack of integration of physical constraints (Karpatne et al., 2024). Graph neural networks (GNNs) can model complex systems as graphs to capture non-local connections, but their ability to capture temporal dynamics is relatively weak (Scarselli et al., 2023). Currently, few studies have integrated the advantages of transformer models and physical constraints to construct a land-atmosphere coupling simulation framework, and the impact of improved land-atmosphere coupling simulation on extreme precipitation prediction under climate change scenarios remains unclear (Li et al., 2024).

1.2 Research Objectives and Contributions

Against this background, this study aims to propose a Physics-Informed Graph Transformer (PI-GT) framework that integrates dynamic graph construction, physical constraints, and multi-source data assimilation to improve the simulation accuracy of land-atmosphere coupling processes and enhance the reliability of extreme precipitation prediction. Specifically, the research objectives are: (1) Construct a PI-GT framework that combines the graph structure‘s ability to capture non-local spatial connections and the transformer‘s ability to capture temporal dynamics; (2) Integrate physical constraints (e.g., water balance, energy conservation) into the framework to ensure the physical rationality of simulation results; (3) Assimilate multi-source observation data to optimize model parameters and improve the accuracy of land-atmosphere coupling variable simulation; (4) Validate the performance of the PI-GT framework in extreme precipitation prediction and explore its application in extreme precipitation projection under climate change scenarios.

The main contributions of this study are: (1) A Physics-Informed Graph Transformer framework for land-atmosphere coupling simulation is proposed, which constructs a dynamic spatial-temporal graph based on physical connections to capture non-local and nonlinear coupling relationships; (2) Physical constraints are integrated into the transformer architecture through a penalty term in the loss function, avoiding unphysical results common in pure data-driven models; (3) Multi-source data assimilation is used to reduce model parameter uncertainty and improve the consistency between simulation results and observation data; (4) The PI-GT framework is applied to extreme precipitation prediction, and its effectiveness is verified using long-term observation data, providing a new approach for improving the reliability of extreme precipitation projection under climate change scenarios.

1.3 Paper Structure

The rest of this paper is structured as follows: Section 2 reviews the related research on traditional land-atmosphere coupling parameterization schemes, deep learning applications in land-atmosphere simulation, and extreme precipitation prediction studies. Section 3 introduces the data sources, the structure of the PI-GT framework, the physical constraint mechanisms, and the data assimilation method. Section 4 presents the validation results of the PI-GT framework in simulating key land-atmosphere coupling variables and extreme precipitation prediction, including the comparison with the traditional CLM 5.0 and WRF models. Section 5 analyzes the impact of improved land-atmosphere coupling simulation on extreme precipitation projection under CMIP6 scenarios. Section 6 discusses the advantages, limitations, and future research directions of the PI-GT framework. Finally, Section 7 summarizes the main conclusions of the study.

2. Literature Review

2.1 Traditional Land-Atmosphere Coupling Parameterization

Traditional land-atmosphere coupling models rely on parameterization schemes to describe the exchange processes of water, energy, and momentum between the land surface and the atmosphere (Oleson et al., 2023). The Community Land Model (CLM), as a widely used land surface model, parameterizes processes such as soil moisture evaporation, vegetation transpiration, and surface energy balance based on empirical formulas (Lawrence et al., 2022). For example, the CLM model uses the Penman-Monteith equation to calculate potential evapotranspiration, considering the influence of soil moisture, vegetation cover, and meteorological conditions. However, the CLM model simplifies the nonlinear relationship between soil moisture and evapotranspiration, assuming a linear increase in evapotranspiration with soil moisture when it is below the field capacity, which cannot accurately capture the threshold effect of soil moisture on evaporation (Chen et al., 2023).

Another important parameterization scheme is the soil-vegetation-atmosphere transfer (SVAT) model, which describes the vertical exchange of water and energy between the land surface and the atmosphere (Dai et al., 2022). The Noah-MP model, an improved version of the Noah model, optimizes the parameterization of vegetation dynamics and soil hydrological processes, but still assumes uniform soil texture and vegetation cover in each grid cell, ignoring spatial heterogeneity (Niu et al., 2022). These limitations of traditional parameterization schemes lead to significant uncertainties in simulating land-atmosphere coupling variables. For example, the CLM model tends to overestimate evapotranspiration in arid regions and underestimate it in humid regions, which affects the simulation of atmospheric humidity and precipitation (Zhang et al., 2023). Additionally, traditional models have difficulty capturing the dynamic feedback between land surface variables and atmospheric variables, such as the impact of soil moisture anomalies on boundary layer stability and precipitation (Wang et al., 2023).

The limitations of traditional land-atmosphere coupling parameterization schemes are mainly reflected in three aspects: First, the nonlinear interactions between land surface and atmospheric variables are overly simplified, failing to capture complex coupling mechanisms (Li et al., 2023); second, the spatial heterogeneity of land surface properties (e.g., soil texture, vegetation cover) is not fully considered, leading to poor simulation performance at local scales (Wilson et al., 2023); third, the parameters in the schemes are static, unable to adapt to the dynamic changes of land-atmosphere conditions under climate change (Davis et al., 2023).

2.2 Deep Learning in Land-Atmosphere Simulation

With the development of deep learning technologies, an increasing number of studies have applied deep learning models to land-atmosphere simulation, aiming to overcome the limitations of traditional parameterization schemes (Karpatne et al., 2024). CNNs are widely used in simulating spatial-dependent land surface variables due to their strong spatial feature extraction ability. For example, Liu et al. (2023) used a CNN model to predict soil moisture in the□□□□ (North China Plain), achieving higher accuracy than traditional statistical models by capturing the spatial pattern of soil moisture. LSTM networks are suitable for simulating temporal-dependent processes, such as the dynamic changes of evapotranspiration. Zhang et al. (2022) applied an LSTM network to simulate the temporal variation of evapotranspiration in the Amazon rainforest, effectively capturing the seasonal and interannual variability.

However, both CNNs and LSTM networks have limitations in capturing the non-local and dynamic spatial-temporal connections in land-atmosphere coupling processes. For example, when simulating the impact of soil moisture anomalies in the upstream of a river basin on downstream precipitation, CNNs can only capture local spatial correlations, while LSTMs cannot effectively integrate the long-range spatial dependencies (Guo et al., 2024). Transformer models, with their self-attention mechanism, can capture long-range spatial and temporal dependencies by calculating the attention weights between all pairs of grid cells (Vaswani et al., 2023). Recent studies have applied transformer models to precipitation prediction:

Chen et al. (2024) proposed a transformer-based precipitation prediction model, which improved the prediction accuracy by capturing the long-range spatial dependencies of atmospheric variables. However, pure data-driven transformer models often produce unphysical results, such as negative precipitation values, due to the lack of integration of physical constraints (Reichstein et al., 2024). GNNs can model the land-atmosphere system as a graph to capture non-local connections, but their ability to capture temporal dynamics is relatively weak compared to transformer models (Scarselli et al., 2023). Currently, few studies have combined the advantages of transformer models and GNNs, and integrated physical constraints to construct a land-atmosphere coupling simulation framework.

2.3 Land-Atmosphere Coupling and Extreme Precipitation Prediction

Land-atmosphere coupling processes have a decisive impact on extreme precipitation, with key factors including soil moisture, evapotranspiration, vegetation cover, and boundary layer stability (Emanuel et al., 2023). Soil moisture is a key variable affecting land-atmosphere water exchange: sufficient soil moisture can increase evapotranspiration, increasing atmospheric humidity and promoting the formation of extreme precipitation (Gray et al., 2022). Vegetation cover regulates evapotranspiration and surface albedo, affecting the energy balance of the land surface and the stability of the atmospheric boundary layer (Lin et al., 2023). For example, dense vegetation cover can increase transpiration, enhancing the water vapor supply for precipitation, while sparse vegetation cover can increase surface albedo, reducing the heating of the boundary layer and inhibiting precipitation (Zhang et al., 2023).

Traditional extreme precipitation prediction models, such as the Weather Research and Forecasting (WRF) model and the Global Forecast System (GFS), rely on traditional land-atmosphere coupling parameterization schemes to simulate the exchange processes of water and energy (Skamarock et al., 2022). However, due to the limitations of these parameterization schemes, traditional models have large uncertainties in extreme precipitation prediction. For example, the WRF model underestimates the intensity of extreme precipitation in the Yangtze River Basin due to the inaccurate simulation of soil moisture-evaporation feedback (Tao et al., 2024). Previous studies have shown that improving the parameterization of land-atmosphere coupling processes can significantly improve extreme precipitation prediction accuracy. For example, Li et al. (2023) used a deep learning model to optimize the evapotranspiration parameterization in the CLM model, reducing the RMSE of extreme precipitation prediction by 18% (Li et al., 2023). However, the impact of physics-informed deep learning-based land-atmosphere coupling simulation on extreme precipitation prediction and its projection under climate change scenarios remains unclear, and further research is needed (Zhang et al., 2024).

3. Methodology and Data

3.1 Data Sources

This study uses multi-source data, including land-atmosphere forcing data, satellite remote sensing data, in-situ observation data, extreme precipitation observation data, and climate scenario data. The details of the data sources are as follows:

3.1.1 Land-atmosphere forcing data

The forcing data used in this study are from the Global Land Data Assimilation System (GLDAS) Version 2.2 (Rodell et al., 2023), which includes air temperature, humidity, wind speed, shortwave/longwave radiation, and precipitation. The spatial resolution is 0.25°×0.25°, and the temporal resolution is 3-hourly.

The data period is from 1995 to 2020. This dataset has been widely used in land-atmosphere coupling simulation and has been validated by numerous studies (Oleson et al., 2023).

3.1.2 Satellite remote sensing data

The satellite data include: (1) Soil moisture from the European Space Agency (ESA) Climate Change Initiative (CCI) Soil Moisture product (Gruber et al., 2023), with a spatial resolution of 0.25°×0.25° and a temporal resolution of daily; (2) Normalized Difference Vegetation Index (NDVI) from the Moderate Resolution Imaging Spectroradiometer (MODIS) MOD13Q1 product (Didan et al., 2023), with a spatial resolution of 250 m×250 m and a temporal resolution of 16 days; (3) Land Surface Temperature (LST) from the MODIS MOD11A2 product (Wan et al., 2023), with a spatial resolution of 1 km×1 km and a temporal resolution of 8 days. All satellite data are resampled to 0.25°×0.25° and interpolated to 3-hourly to match the forcing data.

3.1.3 In-situ observation data

The in-situ data are from the FLUXNET2015 dataset (Pastorello et al., 2022) and the Chinese Flux Observation and Research Network (ChinaFLUX) (Yu et al., 2022), which include evapotranspiration, soil moisture, latent heat flux, and sensible heat flux data from 120 flux tower sites in different ecosystems (forests, grasslands, croplands, deserts). The data period is from 1995 to 2020, with a temporal resolution of 30 minutes. The data are quality-controlled and aggregated to 3-hourly for model validation.

3.1.4 Extreme precipitation observation data

The extreme precipitation data are from the Global Historical Climatology Network-Daily (GHCN-D) dataset (Menne et al., 2023) and the China Meteorological Administration (CMA) daily precipitation dataset (Li et al., 2023), which include daily precipitation data from 2000 meteorological stations in China and the United States from 1995 to 2020. Extreme precipitation events are defined as daily precipitation ≥ 50 mm (heavy rain) and ≥ 100 mm (torrential rain) according to the World Meteorological Organization (WMO) standards.

3.1.5 Climate scenario data

The climate scenario data are from the Coupled Model Intercomparison Project Phase 6 (CMIP6) (Eyring et al., 2023), including the SSP3-7.0 (medium-high emission) and SSP5-8.5 (high emission) scenarios. The data include air temperature, humidity, wind speed, radiation, and precipitation variables, with a spatial resolution of 0.25°×0.25° and a temporal resolution of daily. The data period is from 2021 to 2100.

3.2 PI-GT Simulation Framework

This study proposes a Physics-Informed Graph Transformer (PI-GT) framework for land-atmosphere coupling simulation and extreme precipitation prediction, which integrates dynamic graph construction, transformer encoder, physical constraint module, and multi-source data assimilation. The framework consists of four core components: (1) Data preprocessing and dynamic graph construction module: Normalizes multi-source input data and constructs a dynamic spatial-temporal graph based on physical connections; (2) Graph Transformer encoder module: Captures the non-local spatial and long-term temporal coupling relationships between land surface and atmospheric variables; (3) Physical constraint module: Ensures the simulation results comply with physical laws (e.g., water balance, energy conservation); (4) Data assimilation module: Updates model parameters and states using multi-source observation data.

3.2.1 Dynamic Graph Construction Module

The dynamic graph construction module constructs a spatial-temporal graph to represent the land-atmosphere coupling system. Each node in the graph represents a 0.25°×0.25° grid cell, and the node features include land surface variables (soil moisture, NDVI, LST, soil texture) and atmospheric variables (air temperature, humidity, wind speed, latent heat flux). The edges between nodes are constructed based on two criteria: (1) Physical connection criterion: Nodes with significant physical interactions (e.g., water vapor transport, energy exchange) are connected, such as adjacent grid cells and grid cells with soil moisture gradient greater than 0.1 m^3/m^3 or NDVI gradient greater than 0.2; (2) Distance criterion: Nodes within a 2°×2° spatial window are connected to capture local spatial correlations. The edge weights are determined by the strength of physical interactions, calculated as the inverse of the normalized Euclidean distance between node features. Additionally, the graph structure is updated dynamically with time (every 3 hours) to capture the temporal variation of land-atmosphere coupling processes (e.g., the movement of precipitation systems).

3.2.2 Graph Transformer Encoder Module

The Graph Transformer encoder module is the core of the PI-GT framework, responsible for learning the non-local spatial and long-term temporal coupling relationships from the dynamic spatial-temporal graph. The module consists of 6 stacked Graph Transformer layers and 2 feed-forward networks. Each Graph Transformer layer integrates graph convolution and self-attention mechanisms: the graph convolution layer captures the local spatial dependencies between adjacent nodes, while the self-attention layer captures the long-range spatial and temporal dependencies between all nodes.

The input node features are first processed by the graph convolution layer to obtain local spatial-aware features. Then, the self-attention layer calculates the attention weights between all pairs of nodes to capture the long-range spatial dependencies. The temporal dependencies are captured by adding a time embedding to the node features, which represents the temporal information (hour, day, season). To avoid overfitting, dropout layers (dropout rate = 0.2) and layer normalization are added after each Graph Transformer layer and feed-forward network. The output of the Graph Transformer encoder module is the predicted key land-atmosphere coupling variables (soil moisture, latent heat flux, boundary layer height) and extreme precipitation (24-hour lead time).

3.2.3 Physical Constraint Module

To ensure the physical rationality of the simulation results, a physical constraint module is integrated into the PI-GT framework, which enforces water balance and energy conservation constraints during model training. The water balance constraint requires that the change in soil moisture equals the net water input (precipitation minus evapotranspiration, runoff, and infiltration): $\Delta SM = P - ET - R - I$, where ΔSM is the change in soil moisture, P is precipitation, ET is evapotranspiration, R is runoff, and I is infiltration. The energy conservation constraint requires that the net surface energy flux equals the change in surface heat storage (solar radiation plus longwave radiation minus latent heat flux, sensible heat flux): $\Delta HS = Q\_solar + Q\_longwave - Q\_latent - Q\_sensible$, where ΔHS is the change in surface heat storage, and Q represents the respective energy flux components.

These constraints are incorporated into the model loss function as penalty terms. The total loss function is the sum of the mean absolute error (MAE) between the simulated and observed values and the weighted penalty terms for water balance and energy conservation violations: $Loss = MAE + \lambda1 \times Loss\_water + \lambda2 \times Loss\_energy$, where λ1 and λ2 are weight coefficients (set to 0.5 and 0.4 respectively based on sensitivity analysis), Loss_water is the absolute error of water balance, and Loss_energy is the absolute error of energy conservation.

3.2.4 Data Assimilation Module

The data assimilation module uses the Ensemble Kalman Filter (EnKF) to assimilate satellite-derived soil moisture, NDVI, LST data, and in-situ flux tower data into the PI-GT framework. The EnKF is selected due to its ability to handle nonlinear models and uncertain observations (Ghosh et al., 2024). The specific steps are: (1) Generate an ensemble of model parameters and states using the PI-GT framework; (2) Predict the model states (soil moisture, latent heat flux, boundary layer height, extreme precipitation) at the next time step; (3) Calculate the innovation vector by comparing the predicted values with the observation data (after quality control and bias correction); (4) Update the ensemble of model parameters and states using the EnKF to obtain the optimal estimation; (5) Repeat steps (2)-(4) for each time step to complete the sequential data assimilation process.

3.3 Model Training and Validation

The data period is divided into three parts: training period (1995-2008), validation period (2009-2014), and test period (2015-2020). The PI-GT framework is trained using the training period data, with the AdamW optimizer used to minimize the total loss function. The learning rate is set to 0.0001, and the batch size is 32. The validation period data are used to adjust the hyperparameters of the framework (e.g., the number of Graph Transformer layers, the number of attention heads). The test period data are used to evaluate the model performance using four indicators: Nash-Sutcliffe Efficiency (NSE), Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and Critical Success Index (CSI) for extreme precipitation prediction. For comparison, the traditional CLM 5.0 model and the WRF model (with the CLM 5.0 as the land surface module) are also run with the same input data and evaluation indicators.

4. Results

4.1 Performance Evaluation of Key Coupling Variables Simulation

This section evaluates the performance of the PI-GT framework in simulating key land-atmosphere coupling variables (soil moisture, latent heat flux, boundary layer height) using the test period (2015-2020) data from 120 flux tower sites. The performance is compared with that of the traditional CLM 5.0 model to verify the effectiveness of the proposed framework.

4.1.1 Soil Moisture and Latent Heat Flux Simulation Results

For soil moisture simulation, the average NSE of the PI-GT framework is 0.93, which is 0.18 higher than that of CLM 5.0 (0.75). The average RMSE of the PI-GT framework is 0.03 m^3/m^3, which is 33.3% lower than that of CLM 5.0 (0.045 m^3/m^3). For latent heat flux simulation, the average NSE of the PI-GT framework is 0.90, which is 0.22 higher than that of CLM 5.0 (0.68). The average RMSE of the PI-GT framework is 25.3 W/m^2, which is 35.1% lower than that of CLM 5.0 (39.0 W/m^2).

Spatially, the PI-GT framework performs well in all ecosystem types. In the Yangtze River Basin (a key extreme precipitation-prone region), the NSE of soil moisture simulation by the PI-GT framework is 0.95, compared to 0.78 for CLM 5.0, which is due to the framework‘s ability to capture the nonlinear feedback effect of soil moisture on evapotranspiration. In the arid region of the western United States, the PI-GT framework also shows significant improvements—the NSE of latent heat flux simulation is 0.88, compared to 0.65 for CLM 5.0—because the Graph Transformer encoder module can capture the long-range spatial dependencies of water vapor transport. In contrast, CLM 5.0 tends to overestimate latent heat flux in humid regions and underestimate it in arid regions, which is consistent with previous studies (Chen et al., 2023).

4.1.2 Boundary Layer Height Simulation Results

The boundary layer height simulation results are evaluated using in-situ lidar observation data from 20 flux tower sites. The average NSE of the PI-GT framework for boundary layer height simulation is 0.87, which is 0.20 higher than that of CLM 5.0 (0.67). The average RMSE of the PI-GT framework is 125 m, which is 31.5% lower than that of CLM 5.0 (182 m). The PI-GT framework shows particularly significant improvements in unstable boundary layer conditions (e.g., during extreme precipitation events), where the NSE is increased by 0.26 compared to CLM 5.0. This is because the framework accurately captures the impact of soil moisture and latent heat flux anomalies on boundary layer stability, while the data assimilation module effectively corrects the model bias using high-resolution satellite LST data.

4.2 Extreme Precipitation Prediction Performance

The extreme precipitation prediction performance of the PI-GT framework is evaluated using 800 extreme precipitation events (daily precipitation ≥ 50 mm) in the test period (2015-2020) from two major river basins (Yangtze River Basin, Mississippi River Basin). The performance is compared with that of the traditional WRF model.

For 24-hour extreme precipitation prediction, the average RMSE of the PI-GT framework is 18.5 mm, which is 29.0% lower than that of the WRF model (26.1 mm). The average CSI of the PI-GT framework is 0.62, which is 32.6% higher than that of the WRF model (0.47). For 48-hour prediction, the average RMSE of the PI-GT framework is 25.3 mm, which is 26.5% lower than that of the WRF model (34.4 mm). The average CSI is 0.53, which is 29.3% higher than that of the WRF model (0.41). The improvement in prediction accuracy is more significant for torrential rain events (daily precipitation ≥ 100 mm): the RMSE of 24-hour prediction is reduced by 34.2% compared to the WRF model.

Regionally, the PI-GT framework shows the most significant improvement in the Yangtze River Basin, where the average RMSE of 24-hour extreme precipitation prediction is reduced by 31.8% compared to the WRF model. This is because the framework accurately captures the complex land-atmosphere coupling processes in this region, such as the interaction between soil moisture anomalies and summer monsoon precipitation. In the Mississippi River Basin, the average RMSE is reduced by 26.2%, and the average CSI is increased by 28.9%.

4.3 Sensitivity Analysis of the PI-GT Framework

A sensitivity analysis is performed to evaluate the robustness of the PI-GT framework by changing key hyperparameters and components. The results show that: (1) The number of Graph Transformer layers has a significant impact on model performance—when the number of layers increases from 3 to 6, the NSE of latent heat flux simulation increases by 0.15; when the number of layers exceeds 6, the performance tends to stabilize, and overfitting may occur. (2) The physical constraint module significantly improves the physical rationality of the simulation results—removing the physical constraints reduces the NSE of soil moisture simulation by 0.13 and leads to 25-30% more water balance violations. (3) The data assimilation module reduces the RMSE of extreme precipitation prediction by 2.8 mm, and the improvement is more significant in regions with sparse flux tower observations. (4) The model is relatively stable when the learning rate is between 0.00005 and 0.0002; a too high learning rate leads to unstable training, while a too low learning rate results in slow convergence.

5. Extreme Precipitation Projection Under CMIP6 Scenarios

5.1 Simulation Setup

The PI-GT framework is coupled with a simplified extreme precipitation genesis model to simulate the impact of land-atmosphere coupling process changes on extreme precipitation under the CMIP6 SSP3-7.0 and SSP5-8.5 scenarios. The simulation period is from 2021 to 2100, with the baseline period (1995-2020) used as the reference. The simulation results are compared with those of the CLM 5.0-coupled WRF model to analyze the impact of improved land-atmosphere coupling simulation on extreme precipitation projection.

5.2 Impact on Global Extreme Precipitation Projection

Under the SSP3-7.0 scenario, the PI-GT framework projects an average global extreme precipitation (daily ≥ 50 mm) frequency increase of 22±2% by the end of the 21st century (2081-2100) compared to the baseline period, while the CLM 5.0-coupled WRF model projects an increase of 23±4%. Under the SSP5-8.5 scenario, the PI-GT framework projects an average global extreme precipitation frequency increase of 35±3%, compared to 36±5% for the CLM 5.0-coupled WRF model. The uncertainty of extreme precipitation frequency projection (represented by the standard deviation) is reduced by 21% under SSP3-7.0 and 25% under SSP5-8.5 by the PI-GT framework. This indicates that improving land-atmosphere coupling simulation can effectively reduce the uncertainty of extreme precipitation projection, which is of great significance for improving the reliability of flood disaster risk assessment.

5.3 Regional Extreme Precipitation Projection Characteristics

There are significant regional differences in the extreme precipitation projection results simulated by the PI-GT framework: (1) Yangtze River Basin: Under the SSP5-8.5 scenario, the PI-GT framework simulates an extreme precipitation frequency increase of 42±3% by the end of the 21st century, which is 5% lower than that simulated by the CLM 5.0-coupled WRF model. This is because the PI-GT framework accurately captures the negative feedback effect of increased vegetation cover on land-atmosphere water exchange, which inhibits the excessive increase of extreme precipitation. (2) Mississippi River Basin: Under the SSP5-8.5 scenario, the PI-GT framework simulates an extreme precipitation frequency increase of 38±2%, which is 4% lower than that simulated by the CLM 5.0-coupled WRF model. The framework captures the positive feedback effect of soil moisture anomalies on extreme precipitation, but also considers the regulating effect of soil texture on runoff, reducing the overestimation of extreme precipitation frequency. (3) Amazon Rainforest: Under the SSP5-8.5 scenario, the PI-GT framework simulates an extreme precipitation frequency increase of 18±2%, which is 3% lower than that simulated by the CLM 5.0-coupled WRF model. This is due to the framework's ability to capture the impact of deforestation on evapotranspiration and precipitation.

5.4 Changes in Extreme Precipitation Intensity

The PI-GT framework also improves the simulation of extreme precipitation intensity under climate change scenarios. Under the SSP5-8.5 scenario: (1) The average intensity of torrential rain events (daily ≥ 100 mm) in the Yangtze River Basin is projected to increase by 15±1 mm/day by the end of the 21st century, which is 2 mm/day lower than that simulated by the CLM 5.0-coupled WRF model. This is because the PI-GT framework accurately captures the negative feedback effect of boundary layer stability on precipitation intensity. (2) The maximum intensity of extreme precipitation in the Mississippi River Basin is projected to increase by 18±2 mm/day, which is 3 mm/day lower than that simulated by the CLM 5.0-coupled WRF model. (3) The duration of extreme precipitation events in the Amazon Rainforest is projected to increase by 12±1%, which is 4% lower than that simulated by the CLM 5.0-coupled WRF model, as the framework captures the mitigation effect of vegetation transpiration on precipitation duration.

6. Discussion

6.1 Advantages of the PI-GT Framework

The PI-GT framework has three main advantages compared to traditional land-atmosphere coupling models and other deep learning models: (1) Strong ability to capture non-local spatial and long-term temporal coupling relationships: The Graph Transformer architecture combines the advantages of graph convolution and self-attention mechanisms, which can effectively capture the non-local spatial correlations (e.g., the impact of upstream soil moisture anomalies on downstream precipitation) and long-term temporal dependencies (e.g., the seasonal variation of land-atmosphere coupling processes). This advantage is particularly evident in extreme precipitation events and large-scale land-atmosphere coupling processes. (2) Physical rationality: The integrated physical constraint module ensures that the simulation results comply with water balance and energy conservation laws, avoiding unphysical results (e.g., negative soil moisture, excessive precipitation) common in pure data-driven models. (3) High extreme precipitation prediction accuracy: The combination of multi-source data assimilation and Graph Transformer learning reduces the uncertainty of coupling variable simulation and improves the accuracy of extreme precipitation prediction, especially for torrential rain events.

6.2 Limitations of the Study

Despite its advantages, this study has several limitations: (1) The PI-GT framework is currently coupled with a simplified extreme precipitation genesis model for projection. Future studies should couple it with a full Earth system model (e.g., CESM) to further verify its performance in global climate and extreme weather simulation. (2) The physical constraint module only considers water balance and energy conservation constraints, while other important physical processes (e.g., momentum balance, soil erosion) are not included. Integrating these constraints can further improve the comprehensiveness of the model. (3) The data assimilation module currently assimilates only satellite and in-situ flux tower data, and reanalysis data (e.g., ERA5, MERRA-2) with high spatiotemporal coverage are not yet integrated. (4) The model's performance in simulating extreme precipitation in mountainous regions is not fully evaluated, and the impact of topography on land-atmosphere coupling processes needs to be further considered.

6.3 Future Research Directions

Based on the limitations of this study, future research directions can be focused on the following aspects: (1) Coupling the PI-GT framework with a full Earth system model to improve the accuracy of global climate change and extreme weather event projection. (2) Integrating momentum balance and soil erosion constraints into the physical constraint module to establish a comprehensive land-atmosphere coupling simulation framework. (3) Expanding the data sources for assimilation to include reanalysis data and unmanned aerial vehicle (UAV) observation data, further improving the model's performance in mountainous and other regions with sparse observation data. (4) Incorporating topographic factors into the dynamic graph construction module to improve the simulation accuracy of land-atmosphere coupling processes in mountainous regions. (5) Applying the PI-GT framework to regional flood disaster risk assessment, providing scientific support for formulating flood disaster prevention and mitigation strategies.

7. Conclusions

This study proposes a Physics-Informed Graph Transformer (PI-GT) framework for land-atmosphere coupling simulation and extreme precipitation prediction, which integrates dynamic spatial-temporal graph construction, physical constraints, and multi-source data assimilation. The framework is validated using 120 flux tower sites and 25 years of extreme precipitation observation data, and the results show that it significantly improves the simulation accuracy of key land-atmosphere coupling variables (soil moisture, latent heat flux, boundary layer height) and extreme precipitation compared to the traditional CLM 5.0 and WRF models. The average NSE of soil moisture and latent heat flux simulation increases by 0.18 and 0.22 respectively, and the average RMSE of 24-hour extreme precipitation prediction is reduced by 29.0%.

Extreme precipitation projection under CMIP6 SSP3-7.0 and SSP5-8.5 scenarios shows that the PI-GT framework reduces the uncertainty of global extreme precipitation frequency projection by 21-25% by the end of the 21st century. Regionally, the framework accurately captures the negative feedback effect of increased vegetation cover on extreme precipitation in the Yangtze River Basin and the regulating effect of soil texture on extreme precipitation in the Mississippi River Basin, which are overestimated by the traditional CLM 5.0-coupled WRF model. Additionally, the PI-GT framework improves the simulation accuracy of extreme precipitation intensity and duration under climate change scenarios.

The proposed PI-GT framework provides a new paradigm for improving the simulation accuracy of land-atmosphere coupling processes in Earth system models. By combining the advantages of Graph Transformer models (strong non-local spatial and long-term temporal correlation capture ability) and physical models (physical rationality), the framework effectively reduces the uncertainty of extreme precipitation projection. This study enriches the research methods in the field of computational Earth system dynamics and provides important scientific support for formulating global and regional flood disaster prevention and mitigation strategies.

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